

We may now construct a table of the characters of the classes of C_{3v} contained in each of the representations D_J of R_3 using Eq. 6-15. The resulting character table is shown in Table 6-9. The representations D_J of R_3 may then be decomposed into the irreducible representations of C_{3v} for integral values of J using Eq. 6-14 together with the characters from Table 6-8 to give the results of Table 6-10.

TABLE 6-10 Reduction of $R_3 \rightarrow C_{3v}$ for integral J

J	$R_3 \rightarrow C_{3v}$	Number of Levels
0	${}^1\Gamma_1$	1
1	${}^1\Gamma_2 + {}^2\Gamma_3$	2
2	${}^1\Gamma_1 + 2{}^2\Gamma_3$	3
3	${}^1\Gamma_1 + 2{}^1\Gamma_2 + 2{}^2\Gamma_3$	5
4	$2{}^1\Gamma_1 + {}^1\Gamma_2 + 3{}^2\Gamma_3$	6
5	${}^1\Gamma_1 + 2{}^1\Gamma_2 + 4{}^2\Gamma_3$	7
6	$3{}^1\Gamma_1 + 2{}^1\Gamma_2 + 4{}^2\Gamma_3$	9
7	$2{}^1\Gamma_1 + 3{}^1\Gamma_2 + 5{}^2\Gamma_3$	10
8	$3{}^1\Gamma_1 + 2{}^1\Gamma_2 + 6{}^2\Gamma_3$	11

For half-integer J the characters of the classes of the double group C'_{3v} contained in each of the representations D_J of R_3 are found again using Eq. 6-15. The characters associated with the classes σ_v and $\bar{\sigma}_v$ are all zero, and those associated with the classes \bar{E} and \bar{C}_3 have the same magnitude, but have opposite sign to that of the classes E and C_3 respectively. It is left to the reader to verify that for integer J the representations D_J of R_3 decompose into the irreducible representations of the double group C'_{3v} as shown in Table 6-11. In the absence of magnetic fields or

TABLE 6-11 Reduction of $R_3 \rightarrow C'_{3v}$ for half-integral J

J	$R_3 \rightarrow C'_{3v}$	Number of Levels
$\frac{1}{2}$	${}^2\Gamma_4$	1
$\frac{3}{2}$	$({}^1\Gamma_5 + {}^1\Gamma_6) + {}^2\Gamma_4$	2
$\frac{5}{2}$	$({}^1\Gamma_5 + {}^1\Gamma_6) + 2{}^2\Gamma_4$	3
$\frac{7}{2}$	$({}^1\Gamma_5 + {}^1\Gamma_6) + 3{}^2\Gamma_4$	4
$\frac{9}{2}$	$2({}^1\Gamma_5 + {}^1\Gamma_6) + 3{}^2\Gamma_4$	5
$\frac{11}{2}$	$2({}^1\Gamma_5 + {}^1\Gamma_6) + 4{}^2\Gamma_4$	6
$\frac{13}{2}$	$2({}^1\Gamma_5 + {}^1\Gamma_6) + 5{}^2\Gamma_4$	7
$\frac{15}{2}$	$3({}^1\Gamma_5 + {}^1\Gamma_6) + 5{}^2\Gamma_4$	8

exchange interactions, the levels that transform according to the irreducible representations ${}^1\Gamma_5$ and ${}^1\Gamma_6$ will, according to Kramers' degeneracy

theorem, always appear as degenerate pairs. Tables for the reductions of the irreducible representations D_J of R_3 to the irreducible representations of the thirty-two crystallographic point groups have been given by Koster et al.²⁷²

Runciman²⁷⁶ has considered the general problem of calculating the number of levels a state of a given J will be split into for each of the thirty-two crystallographic point groups and has shown that the point groups may be classified under four headings as follows:

1. Cubic: O_h, O, T_d, T_h, T .
2. Hexagonal: $D_{6h}, D_6, C_{6v}, C_{6h}, C_6, D_{3h}, C_{3h}, D_{3d}, D_3, C_{3v}, S_6, C_3$.
3. Tetragonal: $D_{4h}, D_4, C_{4v}, C_{4h}, C_4, D_{2d}, S_4$.
4. Lower symmetry: $D_{2h}, D_2, C_{2v}, C_{2h}, C_2, C_s, S_2, C_1$.

Then for integral J all the point groups within one of these classes will give rise to the same number of levels as shown in Table 6-12. For

TABLE 6-12 Splittings for integral J

J	0	1	2	3	4	5	6	7	8
Cubic	1	1	2	3	4	4	6	6	7
Hexagonal	1	2	3	5	6	7	9	10	11
Tetragonal	1	2	4	5	7	8	10	11	13
Lower symmetry	1	3	5	7	9	11	13	15	17

half-integral values of J all the groups other than cubic give rise to $J + \frac{1}{2}$ levels as given in Table 6-13. Thus, knowing the symmetry class at the

TABLE 6-13 Splittings for half-integral J

J	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{7}{2}$	$\frac{9}{2}$	$\frac{11}{2}$	$\frac{13}{2}$	$\frac{15}{2}$
Cubic	1	1	2	3	3	4	5	5
All other symmetries	1	2	3	4	5	6	7	8

site of the rare earth ion in a crystal, we can predict readily the number of levels a state of given J will split into. Alternatively, rare earth ions may be used to probe the symmetry of sites in crystals. An interesting example of use of a rare earth ion as a symmetry probe has been given by Oshima et al.,²⁷⁷ who used the fluorescence of Sm^{3+} to study the phase transition in barium titanate at $-80^\circ C$.

6-4 Descending Symmetries

It is sometimes useful to regard a crystal field as being made up of components of decreasing symmetry.^{278, 279} For example, we might consider